



Contribution ID: 52

Type: **Poster**

DMol3/COSMO-RS Prediction of Aqueous Solubility and Reactivity of Selected Azo Dyes: Effect of Global Orbital Cut-off and COSMO Segment Variation

Tuesday, 5 December 2017 12:00 (20 minutes)

HPC content

I made use of the CHPC to get access to the Material Studio license and I also ran all my simulations on the CHPC cluster.

Primary author: Mr WAHAB, Olaide (Department of Applied Chemistry, University of Johannesburg, P. O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa)

Co-authors: Dr GOVENDER, Krishna (Council for Scientific and Industrial Research, Meraka Institute, Centre for High Performance Computing, 15 Lower Hope Road, Rosebank, Cape Town, 7700.); Dr OLASUNKANMI, Lukman (Department of Chemistry, Faculty of Science, Obafemi Awolowo University, Ile-Ife 220005, Nigeria.); Prof. GOVENDER, Penny (Department of Applied Chemistry, University of Johannesburg, P. O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa)

Presenter: Mr WAHAB, Olaide (Department of Applied Chemistry, University of Johannesburg, P. O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa)

Session Classification: Material Science

Track Classification: Materials Science & Physics